

**AFRL-RV-PS-
TM-2011-0001**

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EXTENDED X-RAY ABSORPTION FINE STRUCTURE STUDY OF BOND CONSTRAINTS IN GE-SB-TE ALLOYS

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7 February 2011

Technical Memorandum

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REPORT DOCUMENTATION PAGE

*Form Approved
OMB No. 0704-0188*

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1. REPORT DATE (DD-MM-YY) 07-02-2011	2. REPORT TYPE Technical Memorandum	3. DATES COVERED (From - To) 08-06-2007 – 30-11-2010		
4. TITLE AND SUBTITLE Extended X-ray Absorption Fine Structure Study of Bond Constraints in Ge-Sb-Te Alloys		5a. CONTRACT NUMBER FA9453-07-1-0201		
		5b. GRANT NUMBER		
		5c. PROGRAM ELEMENT NUMBER 62601F		
		5d. PROJECT NUMBER 4846		
		5e. TASK NUMBER		
		5f. WORK UNIT NUMBER 837677		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) North Carolina State University 2701 Sullivan Dr., Ste 240 Raleigh, NC 27695-0001		8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Research Laboratory Space Vehicles Directorate 3550 Aberdeen Ave., SE Kirtland AFB, NM 87117-5776		10. SPONSOR/MONITOR'S ACRONYM(S) AFRL/RVSE		
		11. SPONSOR/MONITOR'S REPORT NUMBER(S) AFRL-RV-PS-TM-2011-0001		
12. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution is unlimited. (377ABW-2011-0146, dtd 10 Feb 2011)				
13. SUPPLEMENTARY NOTES				
14. ABSTRACT In work performed by researchers in the Physics Department at NC State University, studies of the local structure of GeSbTe alloys were studied using Extended X-Ray Absorption Spectroscopy, or EXAFS. Using the spectroscopic capabilities provided by the MCAT line at the Advanced Photon Source at Argonne National Laboratory, examination of the absorption edges of all three elements Ge, Sb and Te were investigated. This effort was de-scoped because AFOSR dropped funding after one year.				
15. SUBJECT TERMS EXAFS, reconfigurable electronics, chalcogenide materials, amorphous semiconductors, GST				
16. SECURITY CLASSIFICATION OF:		17. LIMITATION OF ABSTRACT Unlimited	18. NUMBER OF PAGES 6	19a. NAME OF RESPONSIBLE PERSON Arthur Edwards
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified		19b. TELEPHONE NUMBER (include area code)

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In work performed by researchers in the Physics Department at NC State University, studies of the local structure of GeSbTe alloys were studied using Extended X-Ray Absorption Spectroscopy, or EXAFS. Using the spectroscopic capabilities provided by the MCAT line at the Advanced Photon Source at Argonne National Laboratory, examination of the absorption edges of all three elements Ge, Sb and Te were investigated.

In these studies, principal results involved determination and interpretation of the nearest neighbor numbers N and bond distances r for each species. Results were internally consistent in that the Te nearest neighbor distances NTe-Sb = 2.83 Å and NTe-Ge = 2.62 Å were the same whether measured from the Te atom or the neighboring (Ge or Sb) atom. Co-ordination numbers N likewise agree for all species measured. The proximity of the Sb and Te edges (atomic numbers 51 and 52 respectively) makes it difficult to distinguish Te-Te and Te-Sb bonds, nonetheless several clear distinctions can be made.

In Ge₂Sb₂Te₅ results suggest that the fundamental local units are Ge₂Te₃, Ge₁₇Te₈₃ and Sb₂Te₃ with essentially all Ge bonded in Ge₂Te₃ structures. The Ge₁₇Te₈₃ structures were found to possess considerable Te-Te bonding. Using Bond Constraint Theory, BCT, these data on local bonding configurations allow one to calculate the average number of constraints per atom in Ge₂Sb₂Te₅. In particular the presence of Ge-Ge bonds and the fact that Te bending constraints can be removed indicate an average number of constraints per atom of 2.38 which is close to the ideal number of 2.4 as per the theory of J.C. Phillips and P. Boulchand. At this value, it is argued that one has an ideal balance between local stress without the percolation of stress through the solid matrix.

BCT argues that low coordination results in a floppy material that would allow for easy glass formation but the steric freedom of such a solid would allow for a plethora of defect states. As coordination is increased bond constraint increases and pockets of rigidity begin to grow. When these pockets of rigidity percolate the material become stressed rigid. It is argued that a narrow range of materials between these extremes exists in a so-called intermediate phase of ideal constraints. Material in this regime should be good glass formers and may exhibit reversible photo- or electrically-induced transitions between amorphous and crystalline phases.

Possessed as it is of an ideal number of constraints, Ge₂Sb₂Te₅ is a good glass-former with an ability to make rapid and reversible transitions between the amorphous and crystalline phases. The ideal nature of Ge₂Sb₂Te₅ can also be argued by appealing to this material's position on the Ge-Sb-Te ternary composition diagram. On this diagram, Ge₂Sb₂Te₅ can be argued to be a pseudo-binary because it lies at the intersection of two tie-lines: one connecting GeTe and Sb₂Te₃ and another connecting Te with GeSb.

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